(S)-Ethyl 3-methyl-5-((4aS,8aS)-2,5,5,8a-tetramethyl-3,4,4a,5

Inchi: InChI=1S/C22H38O2/c1-7-24-20(23)15-16(2)9-11-18-17(3)10-12-19-21(4,5)13-8-14-22(1

InchiKey: DLCQYCQEAHRTEG-XWFZLUIHSA-N

Formula: C22H38O2

SMILES: CCOC(=O)CC(C)CCC1=C(C)CCC2C(C)(C)CCCC12C

Mol. weight [g/mol]: 334.54

CAS: 170868-96-9

Physical Properties

Property code	Value	Unit	Source
gf	-36.89	kJ/mol	Joback Method
hf	-581.55	kJ/mol	Joback Method
hfus	28.79	kJ/mol	Joback Method
hvap	72.85	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	6.299		Crippen Method
mcvol	302.260	ml/mol	McGowan Method
pc	1228.56	kPa	Joback Method
rinpol	2310.60		NIST Webbook
rinpol	2310.60		NIST Webbook
tb	814.10	K	Joback Method
tc	1025.66	K	Joback Method
tf	486.02	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.78	J/mol×K	814.10	Joback Method
cpg	1011.06	J/mol×K	849.36	Joback Method
cpg	1034.95	J/mol×K	884.62	Joback Method
cpg	1058.65	J/mol×K	919.88	Joback Method
cpg	1082.37	J/mol×K	955.14	Joback Method
cpg	1106.33	J/mol×K	990.40	Joback Method
cpg	1130.71	J/mol×K	1025.66	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C170868969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume